

Magnetism

1A

2A

3B

4B

5B

6B

7B

8

1B

2B

3A

4A

5A

6A

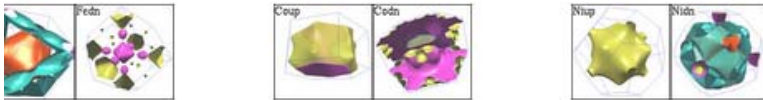
7A

NG

http://www.phys.ufl.edu/fermisurface/periodic_table.html

H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Cu	Zn	Ga	Ge	As	Se	Br	Kr		
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	Xe	
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Lr	Rf	Db	Sg	Bh	Hs	Mt	Uut	Uuq	Uub	Uut	Uuq	Uup	Uub	Uus	Uuo
		•	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	
		••	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	

magnets :



native Structures :



Atomic physics

In atomic physics, the possible values of the magnetic moment of an atom in the direction of the applied field can only take on certain values.

Total angular momentum

$$J = L + S \quad \text{Orbital } L + \text{ spin } S \text{ angular momentum}$$

Magnetic quantum number

$$m_J = -J, -J + 1, \dots, J - 1, J$$

Allowed values of the magnetic moment in the z direction

$$\mu_z = m_j g_J \mu_B$$

Lande g factor \swarrow \nwarrow Bohr magneton

$$g_J \approx \frac{3}{2} + \frac{S(S+1) - L(L+1)}{2J(J+1)}$$

Hund's rules (f - shell)

n	$l_z = 3, 2, 1, 0, -1, -2, -3$	S	$L = \sum l_z $	J
1	↓	1/2	3	5/2
2	↓ ↓	1	5	4
3	↓ ↓ ↓	3/2	6	9/2
4	↓ ↓ ↓ ↓	2	6	4
5	↓ ↓ ↓ ↓ ↓	5/2	5	5/2
6	↓ ↓ ↓ ↓ ↓ ↓	3	3	0
7	↓ ↓ ↓ ↓ ↓ ↓ ↓	7/2	0	7/2
8	↑↑ ↑ ↑ ↑ ↑ ↑	3	3	6
9	↑↑ ↑↑ ↑ ↑ ↑ ↑ ↑	5/2	5	15/2
10	↑↑ ↑↑ ↑↑ ↑ ↑ ↑ ↑ ↑	2	6	8
11	↑↑ ↑↑ ↑↑ ↑↓ ↑ ↑ ↑	3/2	6	15/2
12	↑↑ ↑↑ ↑↓ ↓↓ ↓↓ ↑ ↑	1	5	6
13	↑↑ ↑↓ ↓↓ ↓↓ ↓↓ ↓↓ ↑	1/2	3	7/2
14	↑↑ ↓↓ ↓↓ ↓↓ ↓↓ ↓↓ ↓↓ ↓↓	0	0	0

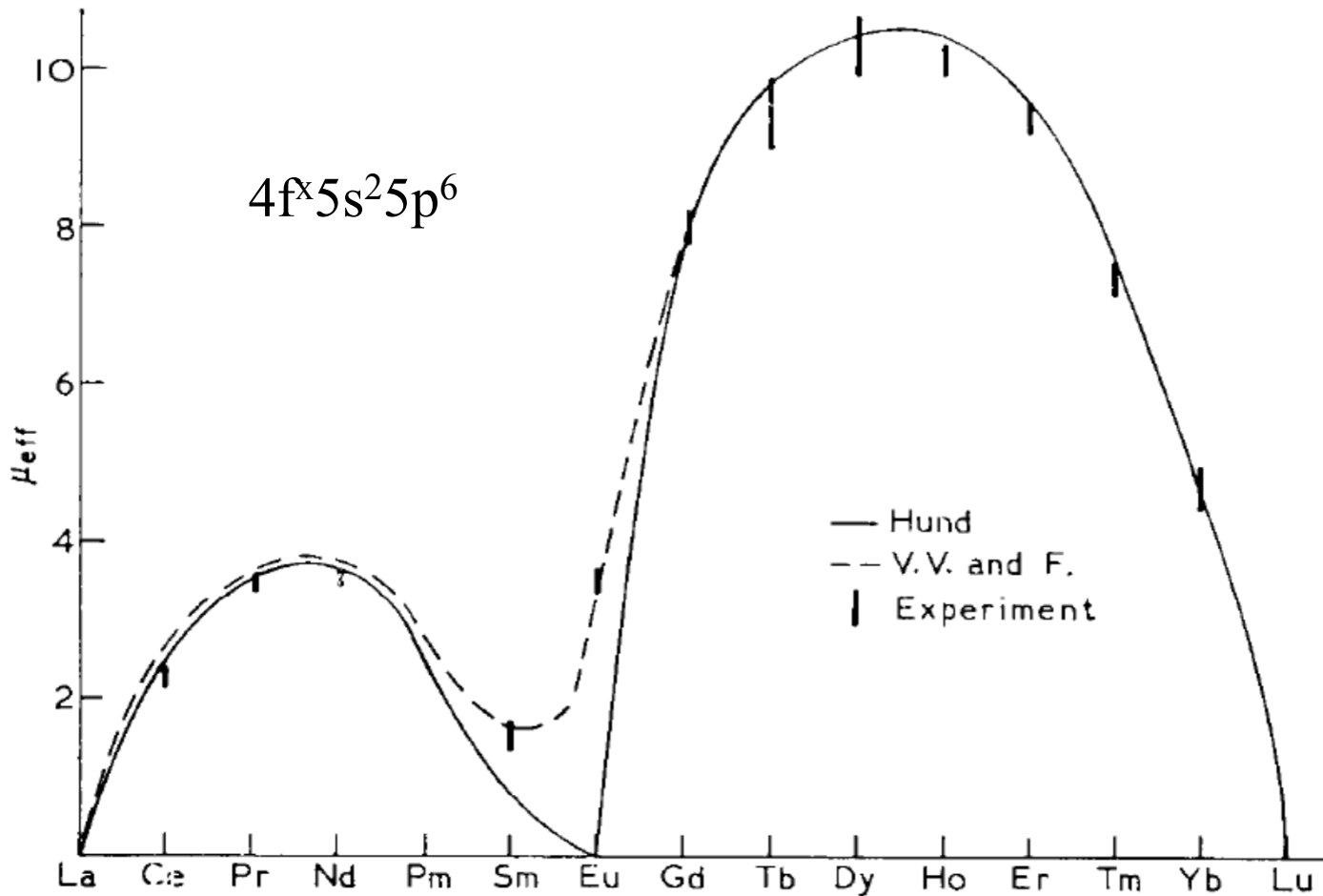
$J = |L - S|$

$J = L + S$

The half filled shell and completely filled shell have zero total angular momentum.

Quantum Mechanics: The Key to Understanding Magnetism

John H. van Vleck



Paramagnetism

In paramagnetism the field aligns local magnetic moments

Paramagnetism due to atomic magnetic moments:

Determine total angular momentum J

Quantized values the magnetic moment in the direction of the field

Use Brillouin functions to describe the field and temperature dependence of the magnetization

Ferromagnetism

Below a critical temperature (called the Curie temperature) a magnetization spontaneously appears in a ferromagnet even in the absence of a magnetic field.

Iron, nickel, and cobalt are ferromagnetic.

Ferromagnetism overcomes the magnetic dipole-dipole interactions. It arises from the Coulomb interactions of the electrons. The energy that is gained when the spins align is called the exchange energy.

Schrödinger equation for two particles

$$-\frac{\hbar^2}{2m}(\nabla_1^2 + \nabla_2^2)\psi + V_1(\vec{r}_1)\psi + V_2(\vec{r}_2)\psi + V_{1,2}(\vec{r}_1, \vec{r}_2)\psi = E\psi$$

$\psi(\vec{r}_1, \vec{r}_2) = \psi_1(\vec{r}_1)\psi_2(\vec{r}_2)$ is a solution to the noninteracting Hamiltonian, $V_{1,2} = 0$

$$\psi_A(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}}(\psi_1(\vec{r}_1)\psi_2(\vec{r}_2) - \psi_1(\vec{r}_2)\psi_2(\vec{r}_1)) \begin{pmatrix} \uparrow\uparrow \\ \frac{1}{\sqrt{2}}(\uparrow\downarrow + \downarrow\uparrow) \\ \downarrow\downarrow \end{pmatrix}$$

$$\psi_S(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}}(\psi_1(\vec{r}_1)\psi_2(\vec{r}_2) + \psi_1(\vec{r}_2)\psi_2(\vec{r}_1)) \frac{1}{\sqrt{2}}(\uparrow(\vec{r}_1)\downarrow(\vec{r}_2) - \downarrow(\vec{r}_1)\uparrow(\vec{r}_2))$$

Exchange (Austauschwechselwirkung)

$$\psi_A(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}}(\psi_1(\vec{r}_1)\psi_2(\vec{r}_2) - \psi_1(\vec{r}_2)\psi_2(\vec{r}_1))$$

$$\begin{aligned} \langle \psi_A | H | \psi_A \rangle &= \frac{1}{2} [\langle \psi_1(\vec{r}_1)\psi_2(\vec{r}_2) | H | \psi_1(\vec{r}_1)\psi_2(\vec{r}_2) \rangle - \langle \psi_1(\vec{r}_1)\psi_2(\vec{r}_2) | H | \psi_1(\vec{r}_2)\psi_2(\vec{r}_1) \rangle \\ &\quad - \langle \psi_1(\vec{r}_2)\psi_2(\vec{r}_1) | H | \psi_1(\vec{r}_1)\psi_2(\vec{r}_2) \rangle + \langle \psi_1(\vec{r}_2)\psi_2(\vec{r}_1) | H | \psi_1(\vec{r}_2)\psi_2(\vec{r}_1) \rangle] \end{aligned}$$

$$\psi_S(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}}(\psi_1(\vec{r}_1)\psi_2(\vec{r}_2) + \psi_1(\vec{r}_2)\psi_2(\vec{r}_1))$$

$$\begin{aligned} \langle \psi_S | H | \psi_S \rangle &= \frac{1}{2} [\langle \psi_1(\vec{r}_1)\psi_2(\vec{r}_2) | H | \psi_1(\vec{r}_1)\psi_2(\vec{r}_2) \rangle + \langle \psi_1(\vec{r}_1)\psi_2(\vec{r}_2) | H | \psi_1(\vec{r}_2)\psi_2(\vec{r}_1) \rangle \\ &\quad + \langle \psi_1(\vec{r}_2)\psi_2(\vec{r}_1) | H | \psi_1(\vec{r}_1)\psi_2(\vec{r}_2) \rangle + \langle \psi_1(\vec{r}_2)\psi_2(\vec{r}_1) | H | \psi_1(\vec{r}_2)\psi_2(\vec{r}_1) \rangle] \end{aligned}$$

The difference in energy between the ψ_A and ψ_S is twice the **exchange energy**.

Exchange

The exchange energy can only be defined when you speak of multi-electron wavefunctions. It is the difference in energy between the symmetric solution and the antisymmetric solution. There is only a difference when the electron-electron term is included. Coulomb repulsion determines the exchange energy.

In ferromagnets, the antisymmetric state has a lower energy. Thus the state with parallel spins has lower energy.

In antiferromagnets, the symmetric state has a lower energy. Neighboring spins are antiparallel.

Ordered states have a lower entropy than free electrons.

Mean field theory (Molekularfeldtheorie)

Heisenberg Hamiltonian $H = -\sum_{i,j} J_{i,j} \vec{S}_i \cdot \vec{S}_j - g \mu_B \vec{B} \cdot \sum_i \vec{S}_i$

Exchange energy

Mean field approximation

$$H_{MF} = \sum_i \vec{S}_i \cdot \left(\sum_{\delta} J_{i,\delta} \langle \vec{S} \rangle + g \mu_B \vec{B} \right)$$

δ sums over the neighbors of spin i

Looks like a magnetic field B_{MF}

$$\vec{B}_{MF} = \frac{1}{g \mu_B} \sum_{\delta} J_{i,\delta} \langle \vec{S} \rangle$$

magnetization $\longrightarrow \vec{M} = g \mu_B \frac{N}{V} \langle \vec{S} \rangle$

eliminate $\langle S \rangle$

Mean field theory

$$\vec{B}_{MF} = \frac{V}{Ng^2\mu_B^2} zJ\vec{M}$$

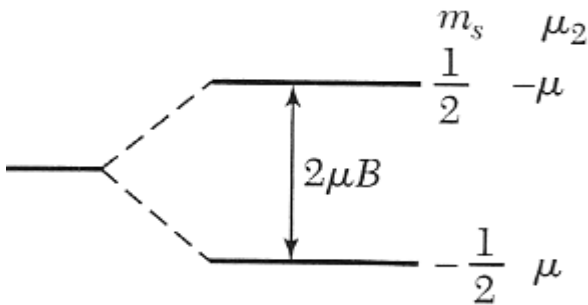
z is the number of nearest neighbors

In mean field, the energy of the spins is

$$E = \pm \frac{1}{2} g \mu_B (B_{MF} + B_a)$$

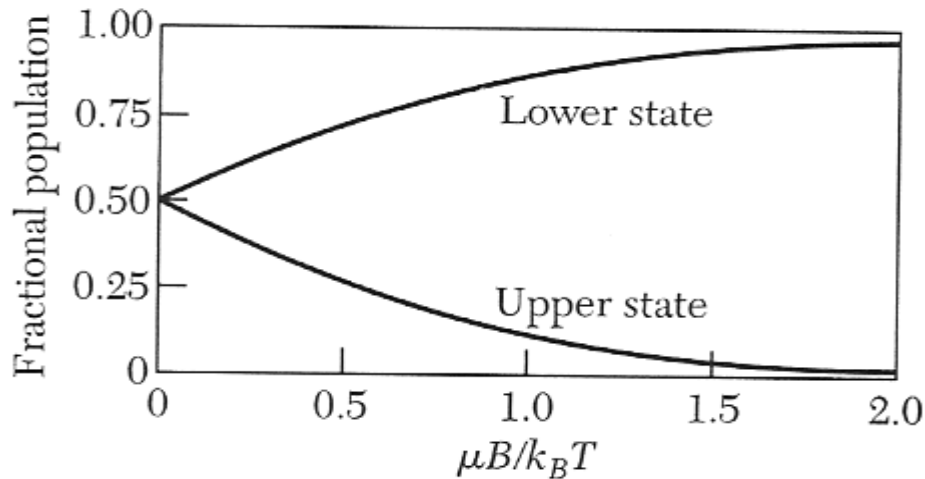
We calculated the populations of the spins in the paramagnetism section

Spin populations



$$\frac{N_1}{N} = \frac{\exp(\mu B / k_B T)}{\exp(\mu B / k_B T) + \exp(-\mu B / k_B T)}$$

$$\frac{N_2}{N} = \frac{\exp(-\mu B / k_B T)}{\exp(\mu B / k_B T) + \exp(-\mu B / k_B T)}$$



$$M = (N_1 - N_2)\mu$$

$$= N \mu \frac{\exp(\mu B / k_B T) - \exp(-\mu B / k_B T)}{\exp(\mu B / k_B T) + \exp(-\mu B / k_B T)}$$

$$= N \mu \tanh\left(\frac{\mu B}{k_B T}\right)$$

Mean field theory

$$M = \frac{1}{2} g \mu_B \frac{N}{V} \tanh \left(\frac{g \mu_B (B_{MF} + B_a)}{2k_B T} \right)$$

For zero applied field

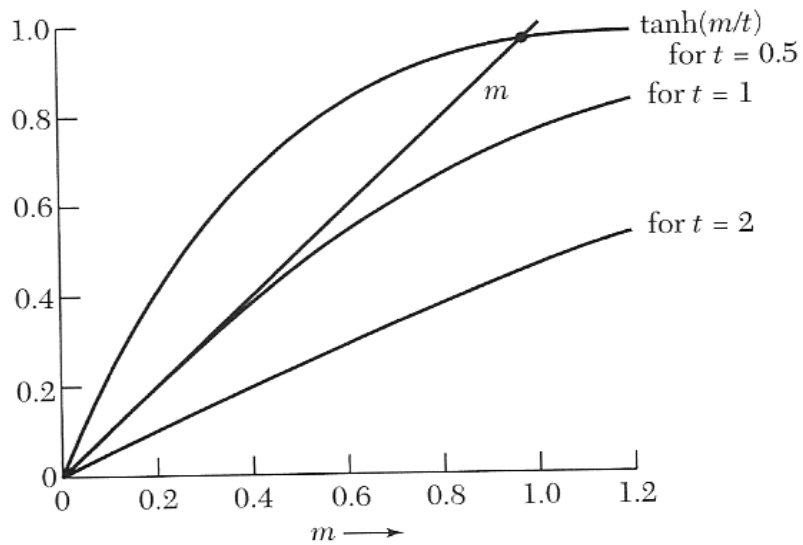
$$M = M_s \tanh \left(\frac{T_c}{T} \frac{M}{M_s} \right)$$

$$M_s = \frac{N}{2V} g \mu_B \quad \text{and} \quad T_c = \frac{z}{4k_B} J$$

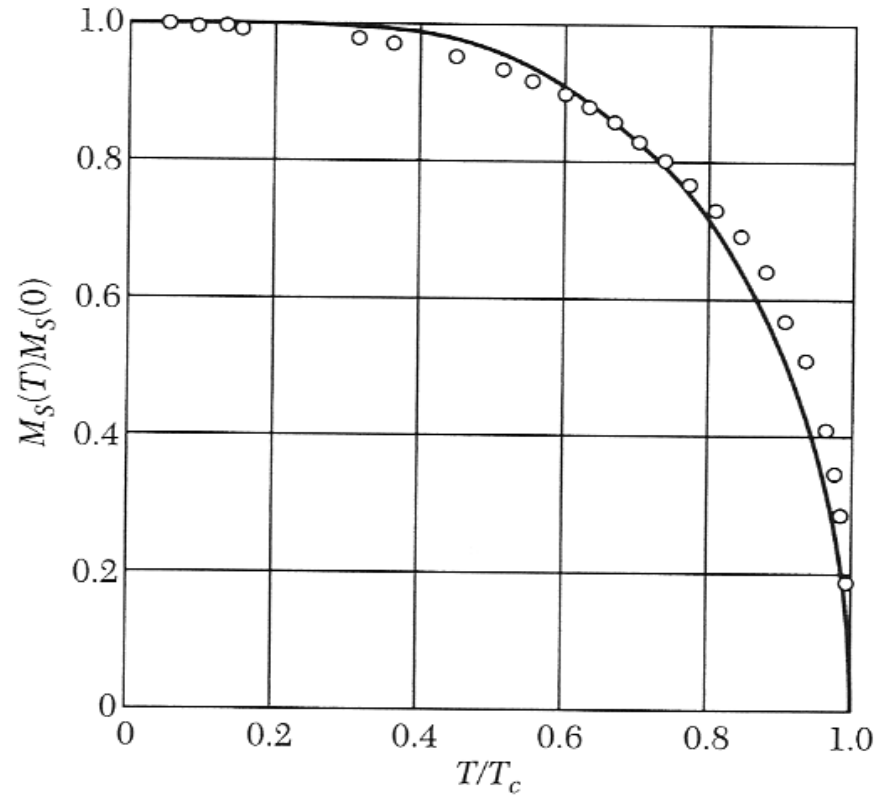
M_s = saturation magnetization T_c = Curie temperature

Mean field theory

$$M = M_s \tanh\left(\frac{T_c}{T} \frac{M}{M_s}\right)$$



$$m = \tanh\left(\frac{m}{t}\right)$$



Experimental points for Ni.

Source: Kittel